

# **When Green Goes Bad:**

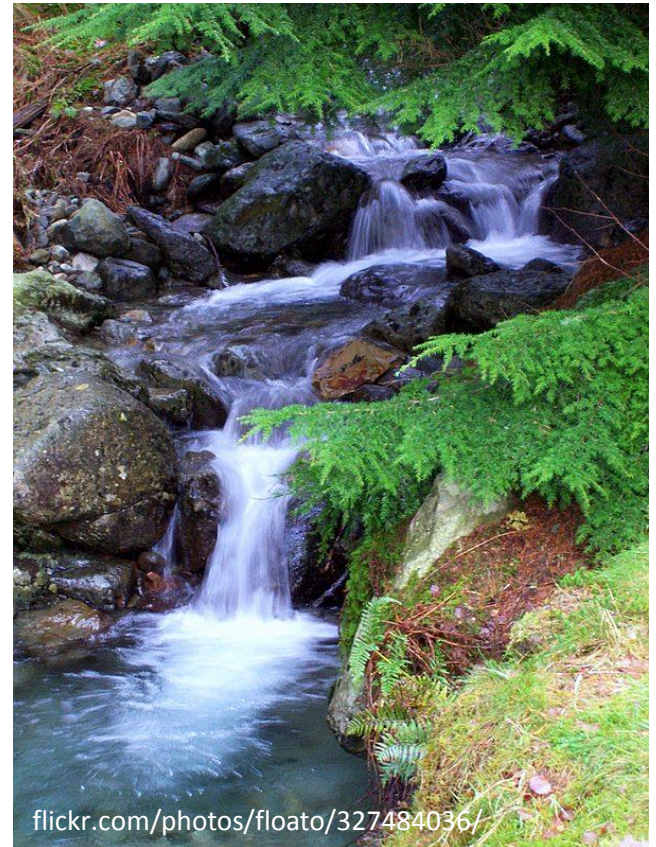
## **A Computational Ecology Approach to a Better Understanding of Cyanobacteria, Nutrients, and Lakes**

Jeff Hollister, Betty Kreakie, Farnaz Nojavan, and W.  
Bryan Milstead

Oct 30, 2014

# Outline

- Introduction to Safe and Sustainable Water Resources (SSWR) Cyanobacteria Project
- Ecological Modelling of Cyanobacteria
  - Machine Learning Approaches
  - Bayesian Approaches
- The Role of Open Science in our Research
- Recent news – N.E. Monitoring (Thanks Hilary Snook!)

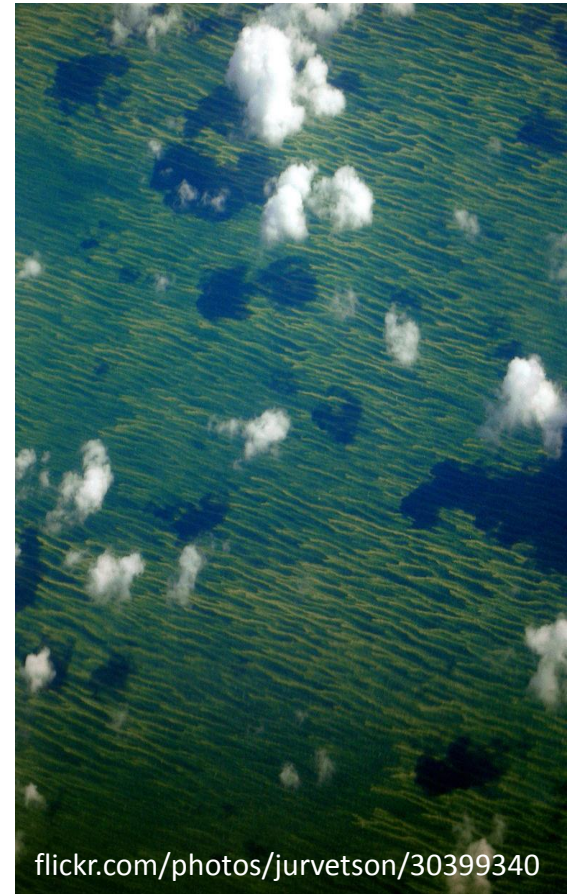


# Introduction



# Cyanobacteria

- “Bluegreen Algae”
- Photosynthetic bacteria
- Found in fresh and salt water
- Amazing diversity
- Many can fix nitrogen
- Resting spores
- Mobile – can harvest nutrients from sediments
- Produce over 80 known toxins



[flickr.com/photos/jurvetson/30399340](https://www.flickr.com/photos/jurvetson/30399340)

# Cyanobacteria Blooms

- Human and Animal Health Risks
- Hypoxia and Fish Kills
- Water Treatment Costs
- Lake Aesthetics –Clarity & Smell
- Quality of Life
  - Recreational Opportunities
  - Property Values
  - Tax Revenues
  - Employment



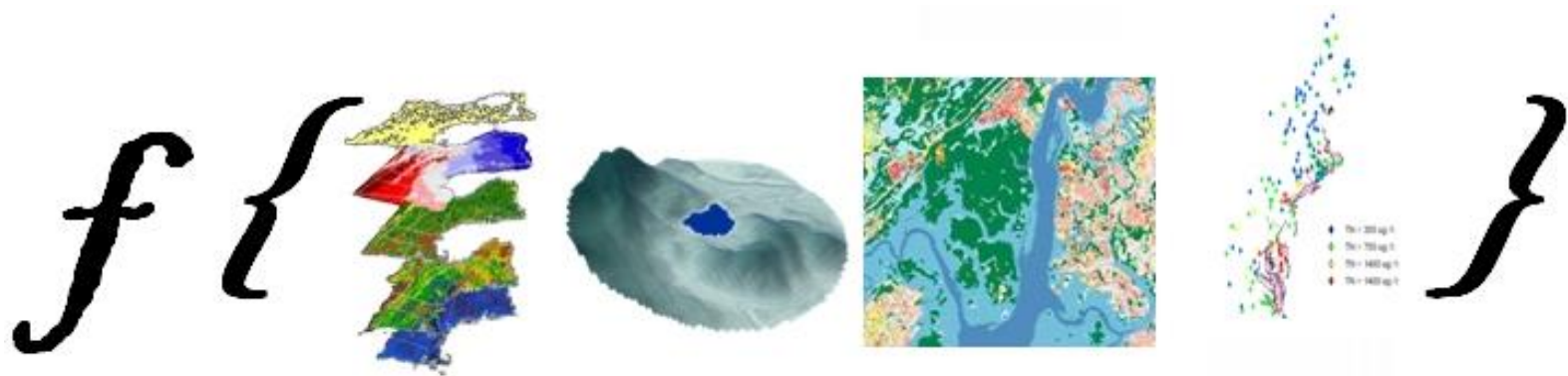
## Cyanobacteria, nutrients, and land use - a nexus for sustainable water resources and human health protection

- **Ecology:** Develop predictive models to relate nutrient loads, land use/land cover, socioeconomic factors, and climate to the frequency, location, and severity of cyanobacterial blooms in lakes of the United States  
Contact: Jeff Hollister and Betty Kreakie
- **Toxicology:** Clarify cyanotoxin effects on mammalian endpoints and exposure biomarker identification for human health risk assessment  
Contact: Neil Chernoff
- **Epidemiology:** Characterize cyanotoxin occurrence and nutrient concentrations in US surface waters. Analyses includes assessing risk to human health via multiple exposure scenarios to recreational and drinking waters  
Contact: Betsy Hilborn
- **Remote Sensing:** Describe the retrieval of chlorophyll a concentrations, and water clarity from airborne hyperspectral data and predictions of changes in trophic status in Northeastern Lakes and Reservoirs  
Contact: Darryl Keith

# Ecological Modelling



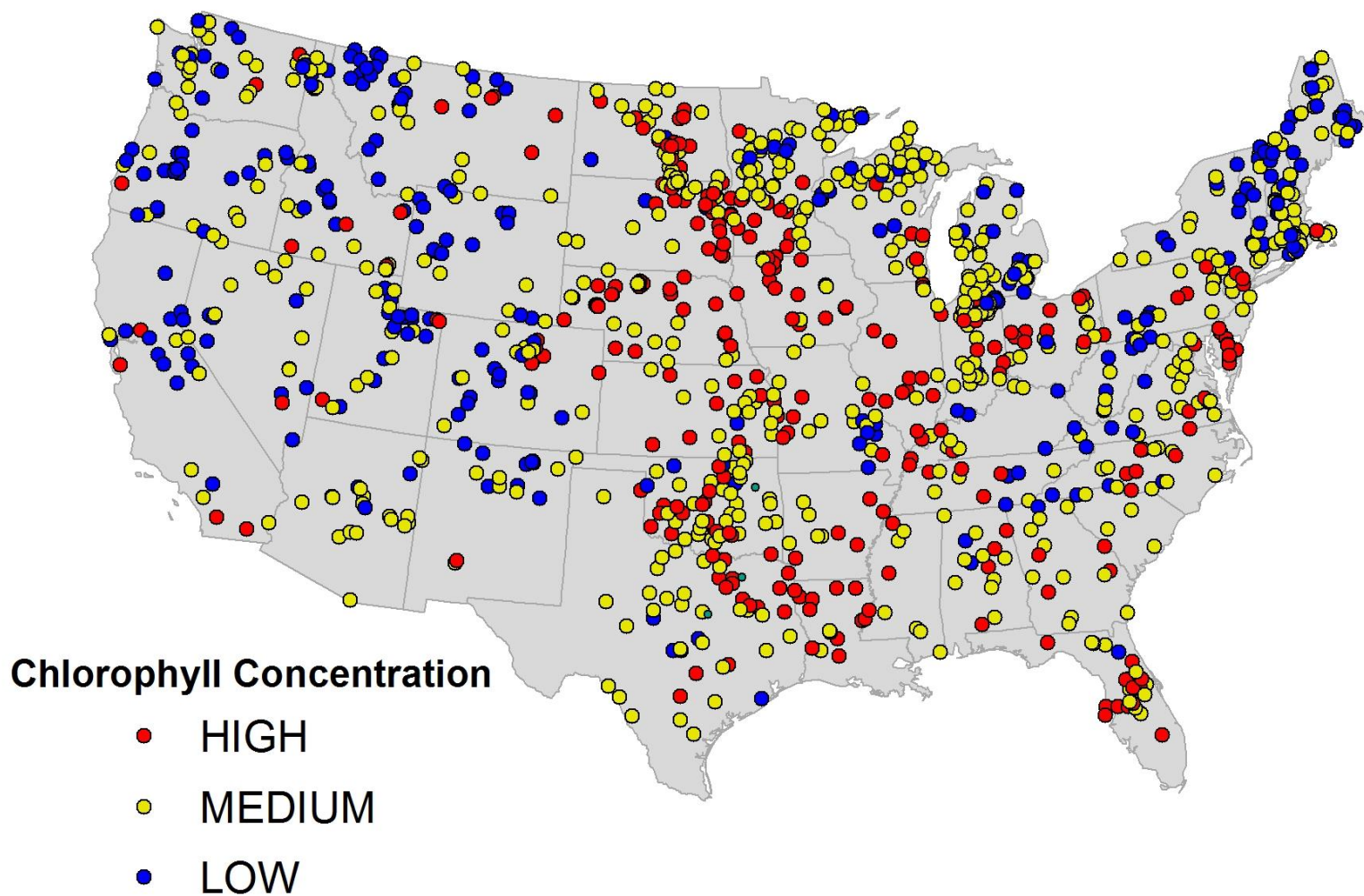
“We are trying to combine what we know from field data, what we know from modeled data, and what we (think) we know about cyanobacteria and create predictive models of the probability of bloom events.”

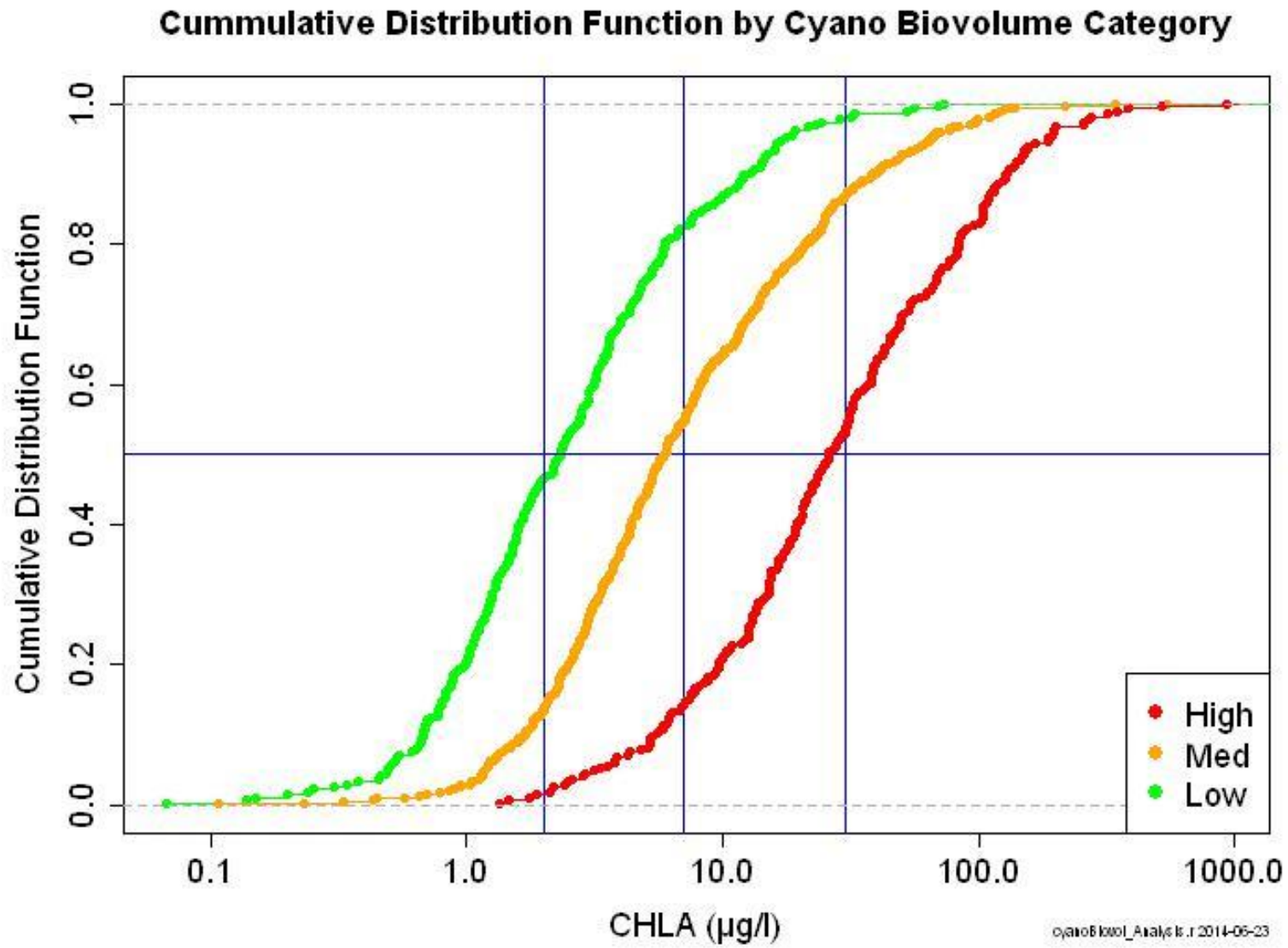


# National Lake Assessment (NLA)

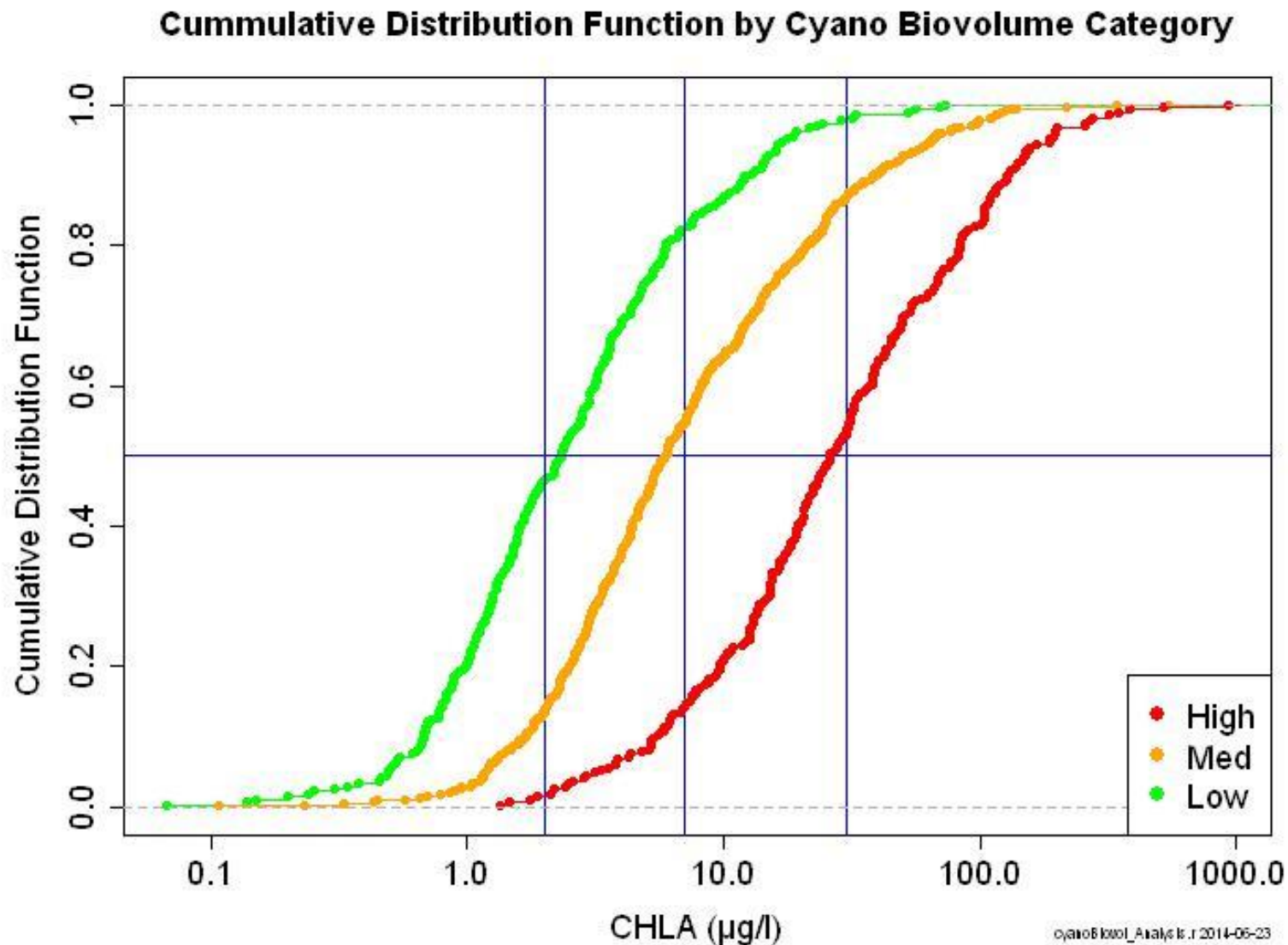
- Spatially balanced, probabilistic sample of 1000+ lakes
- Developed to provide inference on the condition of the lakes in the contiguous United States at the national and ecoregional level
- Includes freshwater lakes greater than 4 hectares (excluding Great Lakes and Great Salt Lake) and deeper than 1 meter
- First Survey in 2007; Second in 2012, Third planned for 2017.

# Map of 2007 NLA Samples



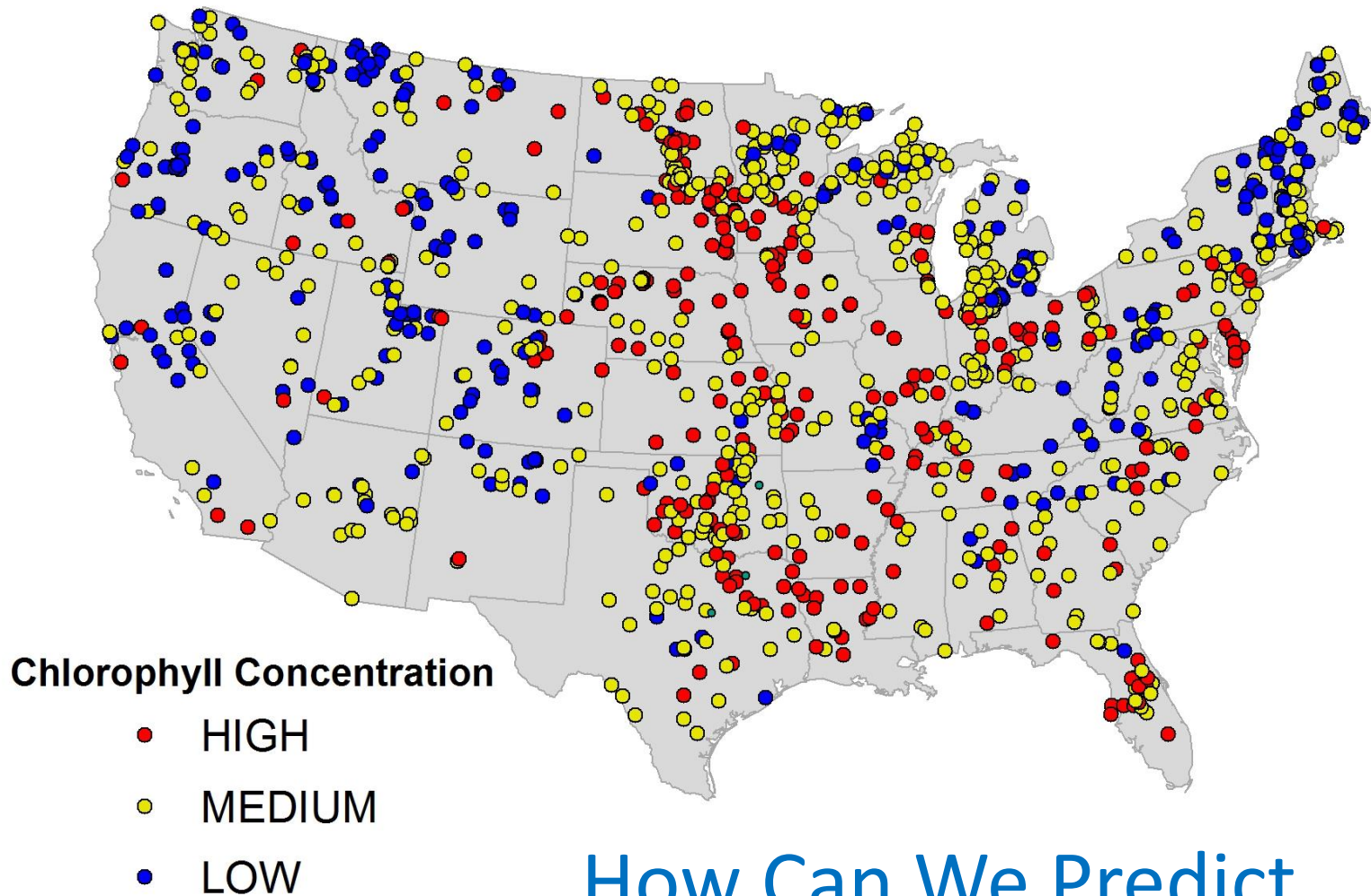


Biovolumes from Lester Yuan (EPA OW) and Beaulieu et al. 2013. Nutrients and water temperature are significant predictors of cyanobacterial biomass in a 1147 lakes dataset. L&O 58:1736-1746.



**Assumption: We can use *Chl a* as a proxy for cyanobacteria biomass & ...**

# Map of 2007 NLA Samples

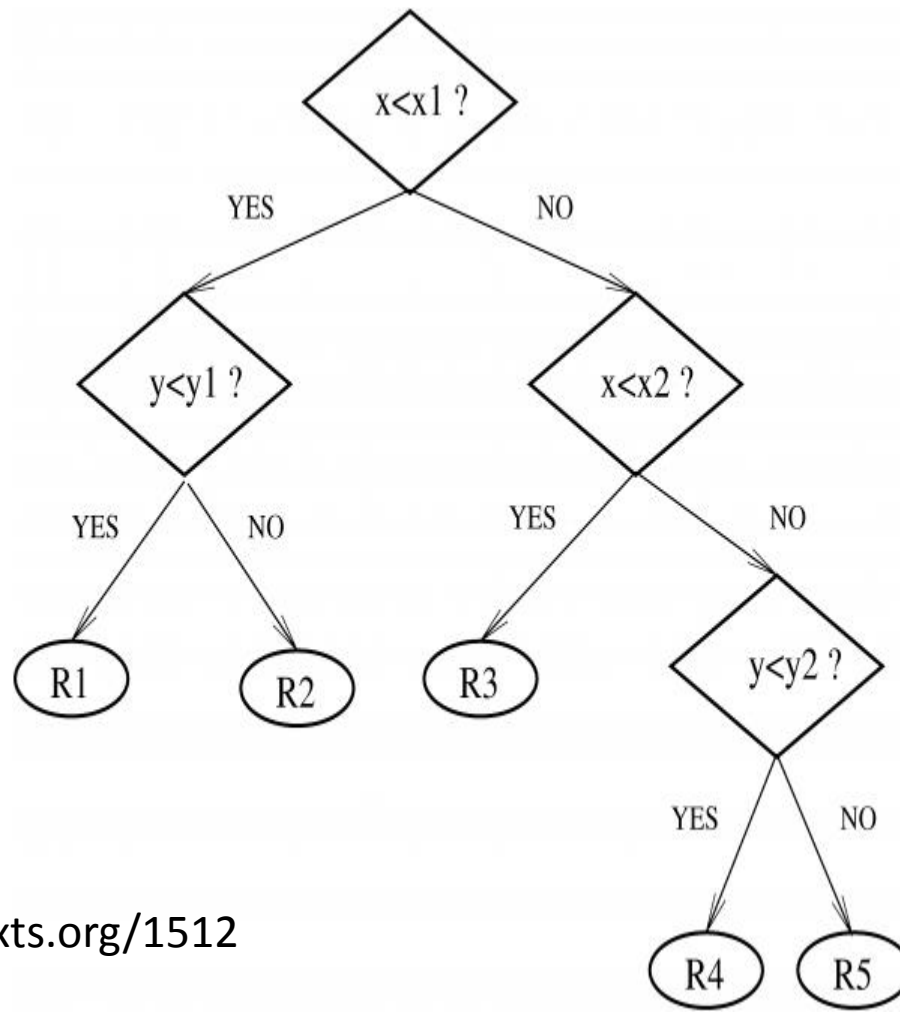


How Can We Predict  
*Chl a* Class?

# Random Forest:

Definition 1.1. A random forest is a classifier consisting of a collection of tree-structured classifiers  $\{h(x, \Theta_k), k = 1, \dots\}$  where the  $\{\Theta_k\}$  are independent identically distributed random vectors and each tree casts a unit vote for the most popular class at input  $x$ .

# CART Model: Classification and Regression Trees



# Random Forest

- Can throw any kind of data at it
  - Included highly correlated variables and NAs
- Can not over fit
  - No weird pruning rules
- Measures of variable importance
- Model verification build directly into the algorithm
- Computationally fast and easy to code
  - Even with very large data sets

# Summary of Random Forest

- Select training data ( $\sim 2/3$ ) with replacement for each tree
- Randomly select subset of variables
  - Actually done for each split
- Make a tree
- Record Out-Of-Bag (OOB) errors
- Permute variables
- Record altered OOB
- Repeat 10,000 times

**\*\*Each tree votes for a classification**

# Random Forest Analysis

## Response Variable

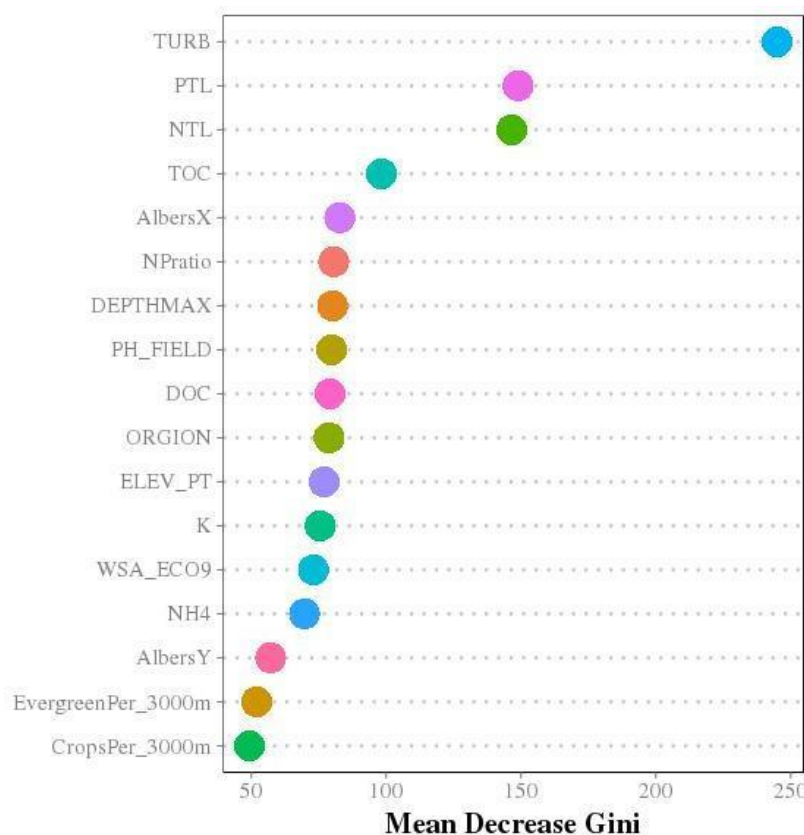
- Chlorophyll a Category

## Predictor Variables (WQ)

- Geographic (5)
- Morphometry (14)
- NLCD 3km (17)
- Water Quality (34)
- Other (2)

# Random Forest Analysis

## Selected WQ Predictors

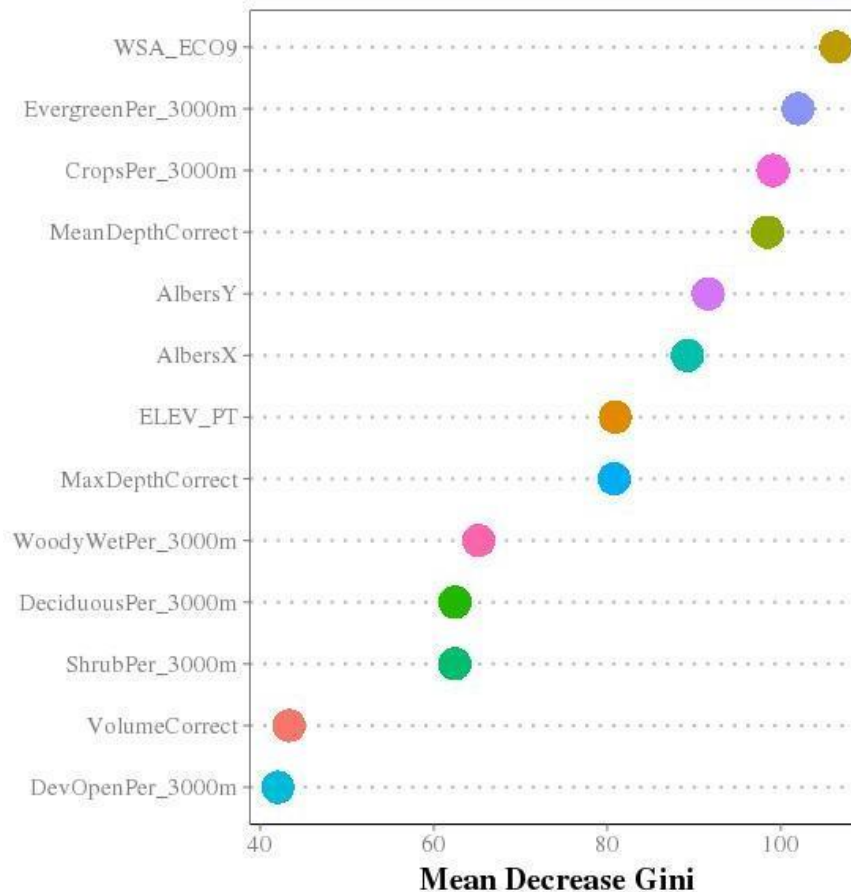


**Out of Bag Error Rate: 21%**

# Random Forest Analysis

- Water quality data  
difficult/expensive to obtain
- What if we just use the GIS  
ready predictors to assign *Chl a*  
category?

# Random Forest Analysis Selected GIS Predictors



**Out of Bag Error Rate: 32%**

# Random Forest Modelling

## WQ Predictors

VARIABLE	PERCENT
K	1.00
NPratio	1.00
NTL	1.00
PTL	1.00
TOC	1.00
TURB	1.00
WSA_ECO9	1.00
ORGION	0.46
DOC	0.21
DEPTHMAX	0.06

**OOB Error Rate: 21%**

## GIS Predictors

VARIABLE	PERCENT
AlbersX	1.00
CropsPer_3000m	1.00
EvergreenPer_3000m	1.00
WSA_ECO9	1.00
MeanDepthCorrect	0.99
AlbersY	0.40
ELEV_PT	0.04
MaxDepthCorrect	0.01

**OOB Error Rate: 32%**

# Future Modelling Efforts

- Explore temporal dynamics and phytoplankton community turnover using a long-term regional data set
- Bayesian forecasting of predicted cyanobacteria bloom risk for lakes in the continental United States
- Develop regional models based on citizen science data (e.g. URI Watershed Watch Data)

# Water Quality Modeling Approaches

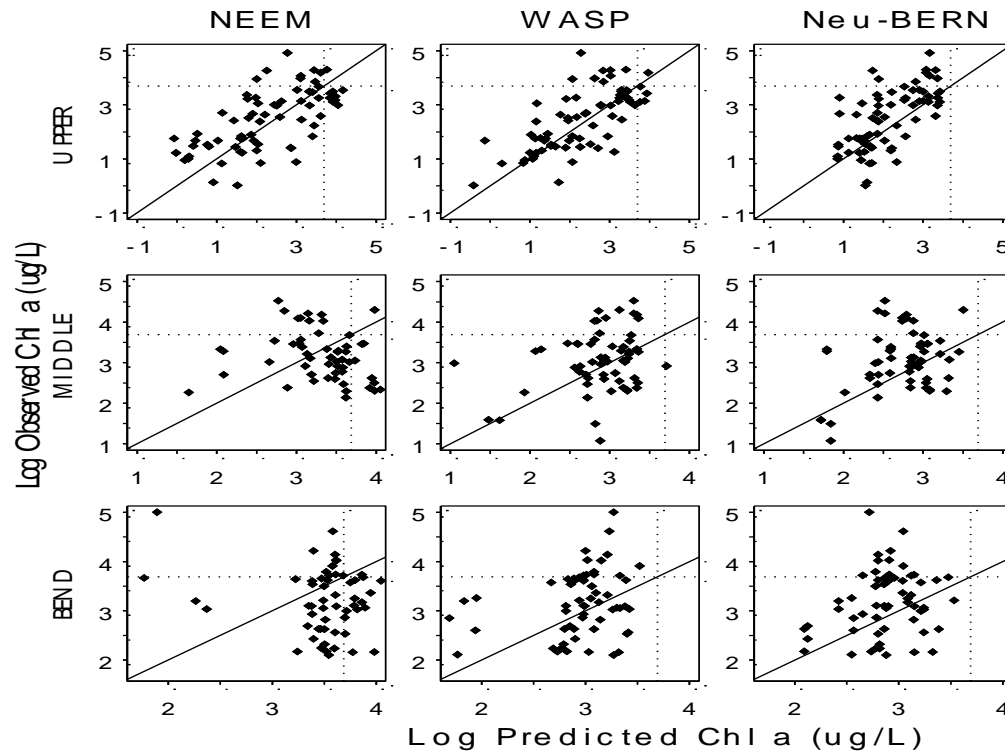
- Process-based models, Deductive reasoning
  - Conceptually dividing a system into subsystems
  - Equations are derived based on existing knowledge and general laws of physics
  - Solving equations for all subsystems together
  - Box-and-arrow charts plus differential equations
- Statistical models, Inductive reasoning
  - Statistical models are mostly driven by data
  - Data – often limited to a specific region (local or subregion)
  - We usually don't combine subsystem models
  - Statistical modeling often does not incorporate existing knowledge – we reinvent the wheel every time we have a new data set.

# Model Updating

## Adaptive Management

- Continuous observation of the ecosystem to gauge the impact of policies and management actions
- Communicating the ecosystem's status with policy makers and managers
- Updating the management actions and recommendation

# High Prediction Uncertainty



Stow et al., 2003, Comparison of Estuarine Water Quality Models for Total Maximum Daily Load Development in Neuse River Estuary

# Quantifying Uncertainty

## Sources of Uncertainty

- Natural ecosystem variability
- Current knowledge of environmental processes
- Model structure uncertainty
- Data and observation (e.g., observation error, missing data)
- Computational restrictions

# Other Considerations

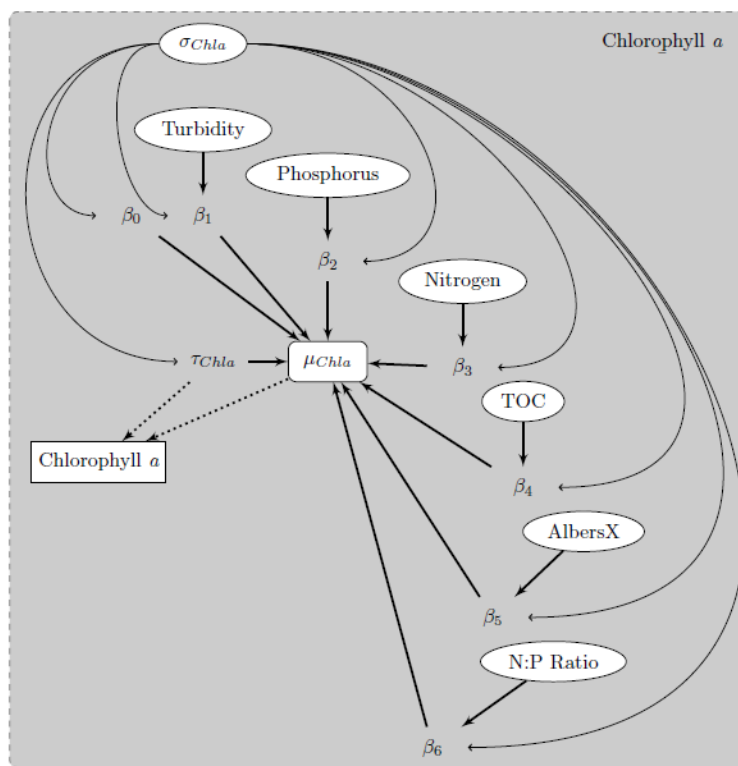
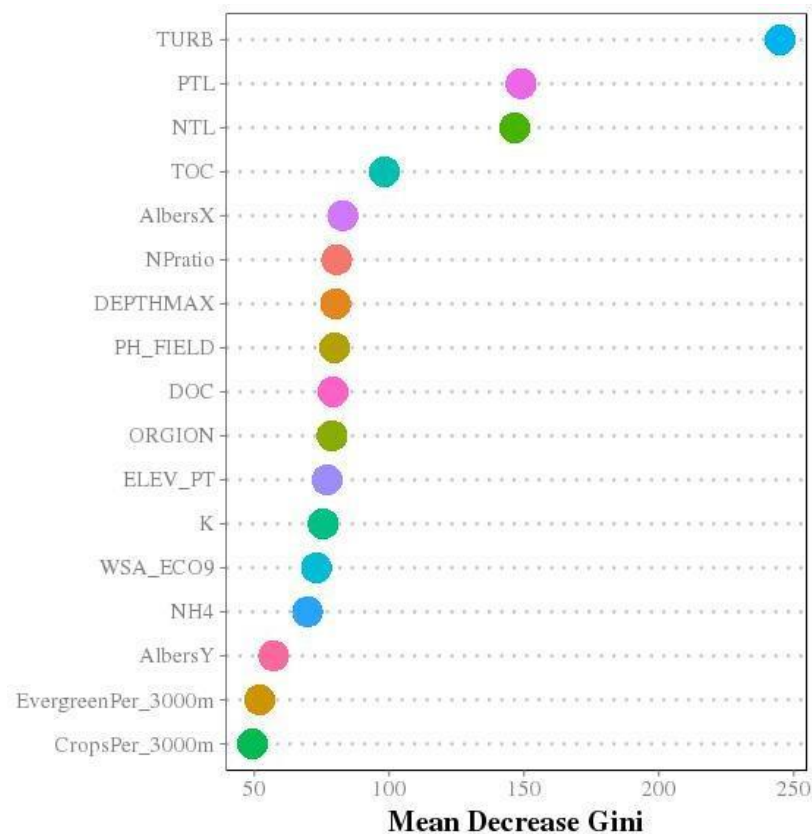
- Small/incomplete data set accommodation
- Visual interface – Communication

# Network-based Bayesian Model

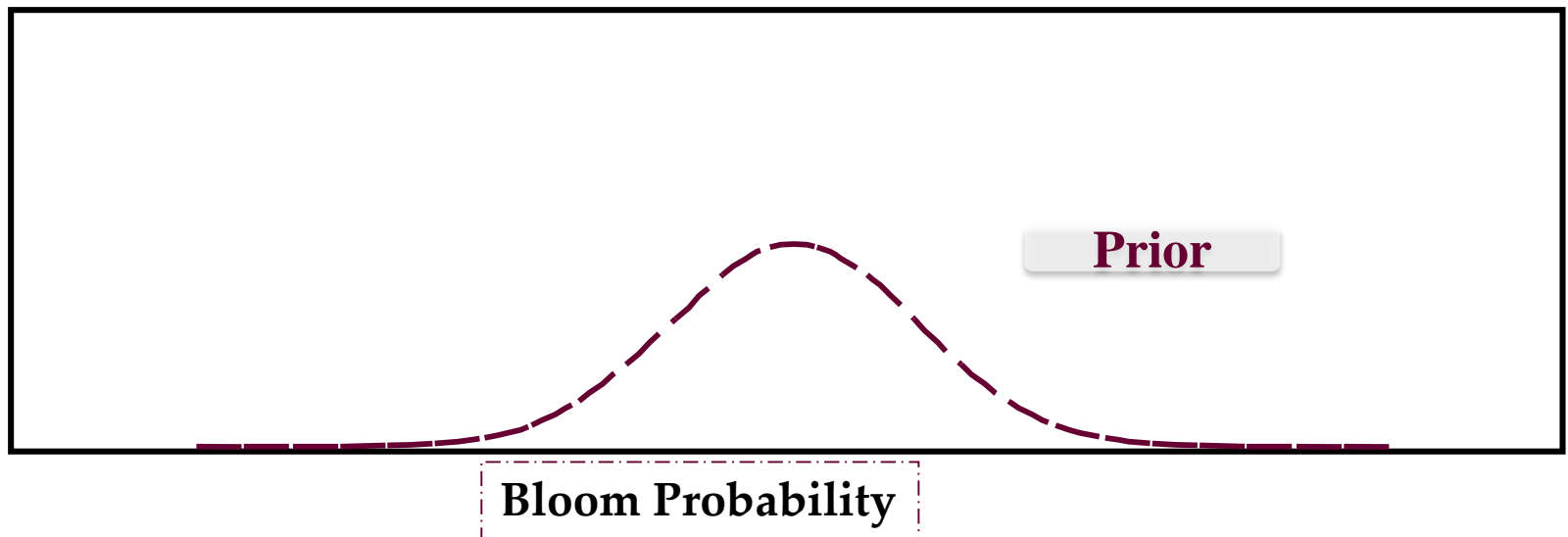
## Model Formulation

- Establishing cause-effect diagram using biological/ecological knowledge (box-and-arrow charts)
- Quantifying the links
- Model updating

# Proposed Network-based Bayesian Model



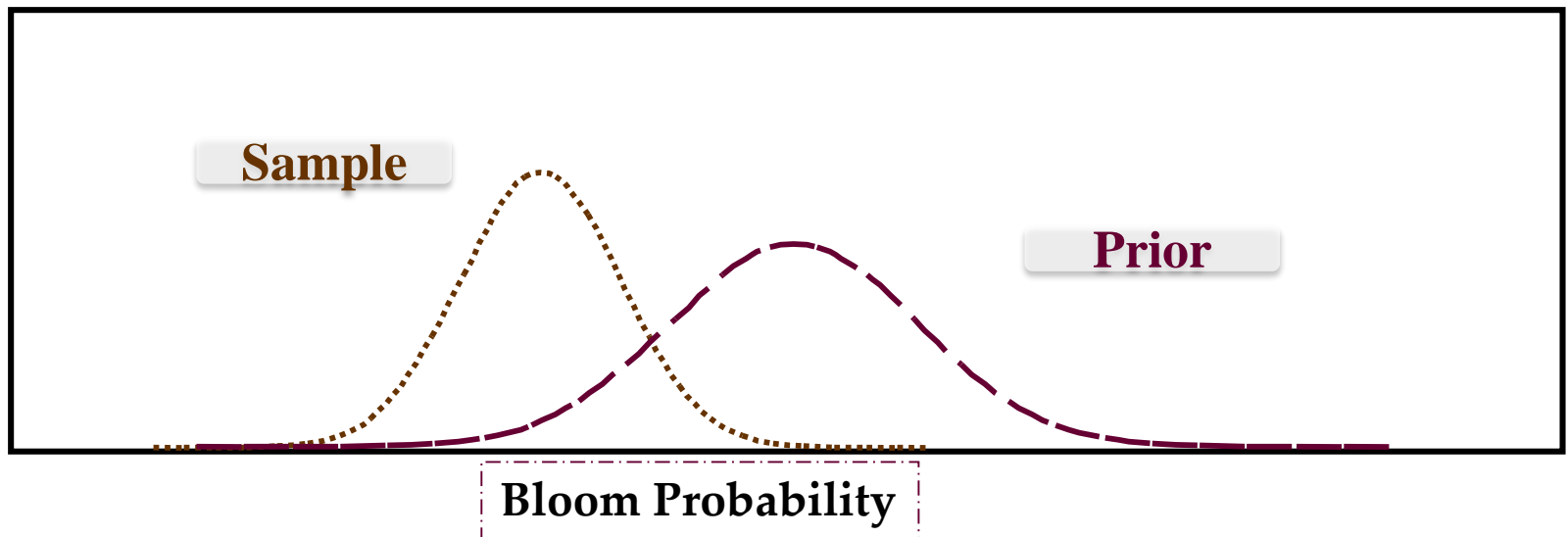
# Model Evaluation & Updating



- Prior: 2007 NLA data set
- Likelihood: 2012 NLA data set

# Model Evaluation & Updating

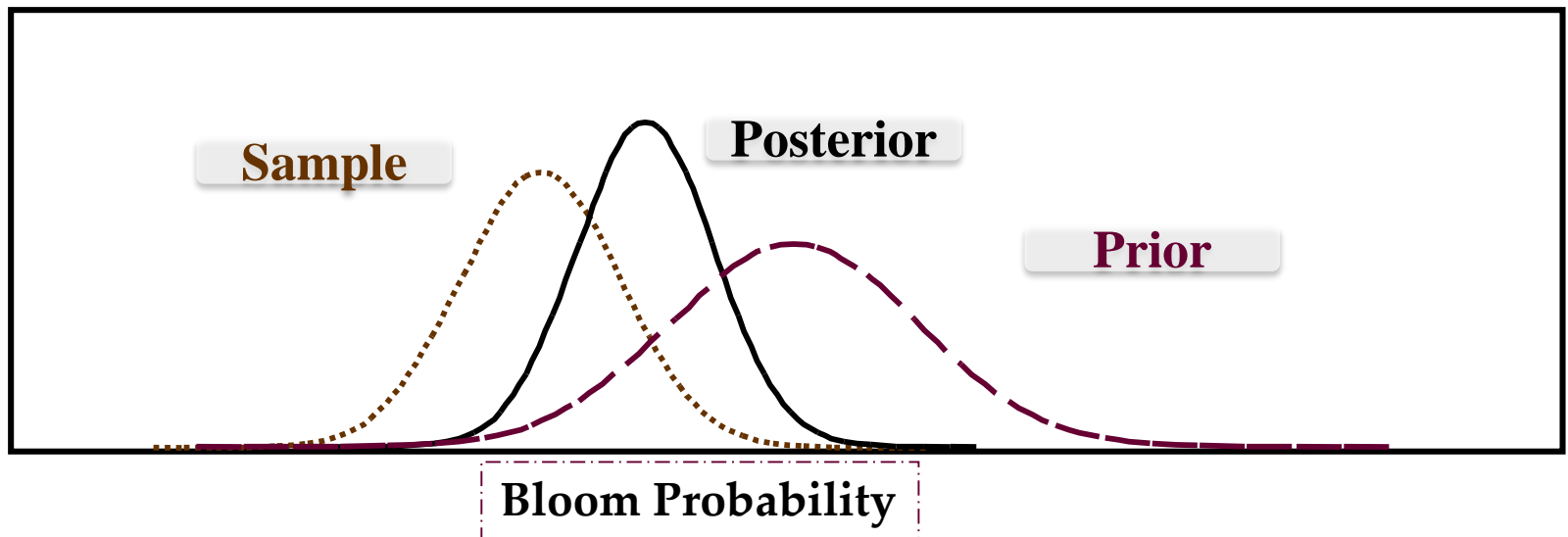
Prior  $\otimes$  Likelihood



- Prior: 2007 NLA data set
- Likelihood: 2012 NLA data set

# Model Evaluation & Updating

Posterior  $\propto$  Prior  $\otimes$  Likelihood

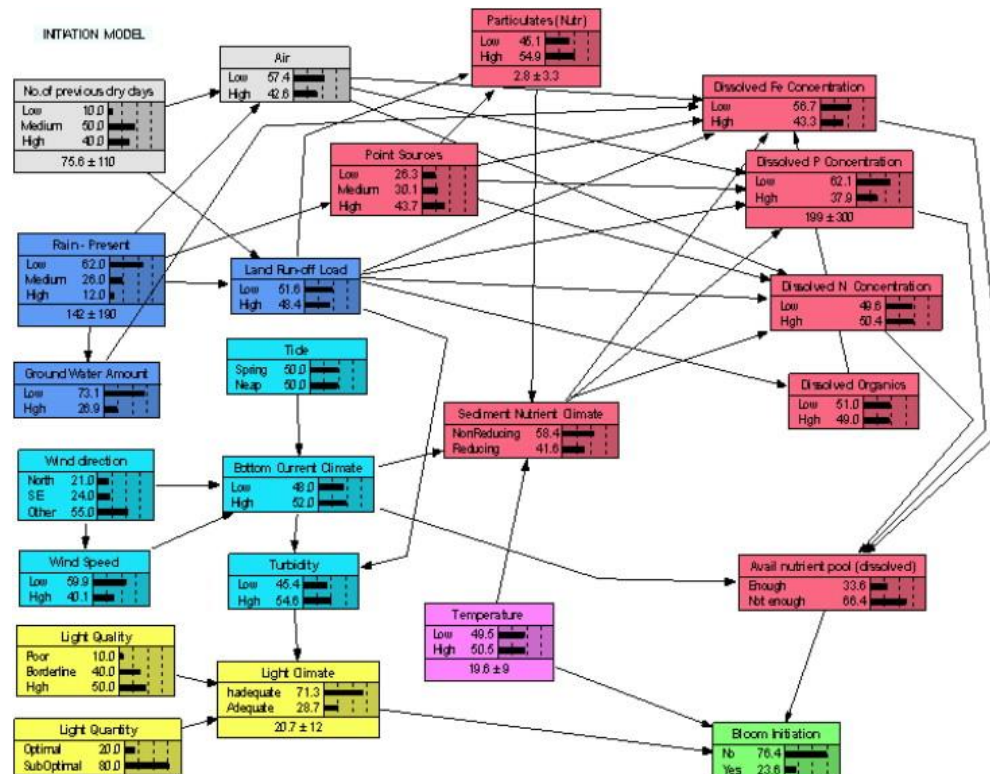


- Prior: 2007 NLA data set
- Likelihood: 2012 NLA data set

# Benefit of Network-based Modeling

- Comprehensive – summarizing all available information
- Flexibility – both empirical models and mechanistic models can be part of a network model
- Updating – over space and time
- A starting point – no need to wait for all necessary information

# Previous Applications (1)



Johnson et al., 2010, An Integrated Bayesian Network approach to *Lyngbya majuscula* bloom initiation

## Previous Applications (2)

Using the observational data sampled during the growing season in 2007–2011, a Bayesian hurdle Poisson model was developed to predict cyanobacteria abundance in lake Paldang, South Korea.

# Open Science

# What is Open Science?

- Many Flavors
- But many agree on:
  - Openness and transparency
  - free access to code, data, publications
  - repeatable
  - reusable
  - web enabled
  - degrees of openness

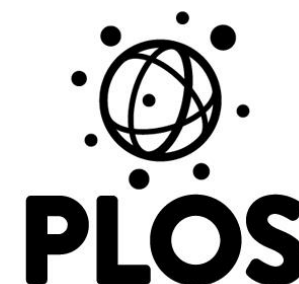


\*See details of definition from a question I posed to twitter at:

<https://storify.com/jholist/what-is-the-definition-of-open-science>

# Why Open Science?

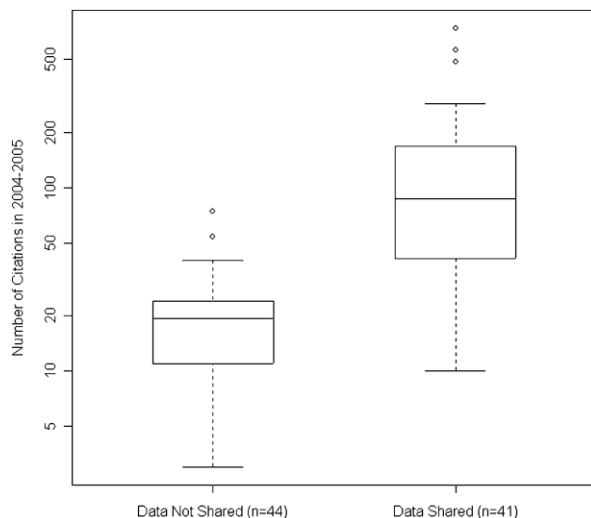
- Expected and/or required
  - Increasing Access to the Results of Federally Funded Scientific Research
    - John Holdren, Director, White House OSTP
    - Feb 2013
  - NSF
  - Publishers
    - #PLOSfail/#PLOSwin
    - [Carly Strasser at DATA PUB](#)



# Why Open Science?

- Benefits

- Open Data = More citations ([Piwowar et al. 2007](#))
- Up-to-date statistics on readership (e.g [PLOS ALM](#))
- Accelerates research and discoveries (e.g. [Woelfle et al. 2011](#))



[Piwowar et al. 2007](#)



[ImpactStory Metrics](#)

# Why Open Science?

- It keeps us honest
- Prevents this:



# Why Open Science?

- Hot off the press:
  - Weecology Blog: [“Sharing in Science: my full reply to Eli Kintisch”](#)
  - Living in an Ivory Basement: [“Thoughts on open science – my response to Eli Kintisch”](#)
  - Science Careers Article by Eli Kintisch: [Give, and It Will Be Given to You](#)

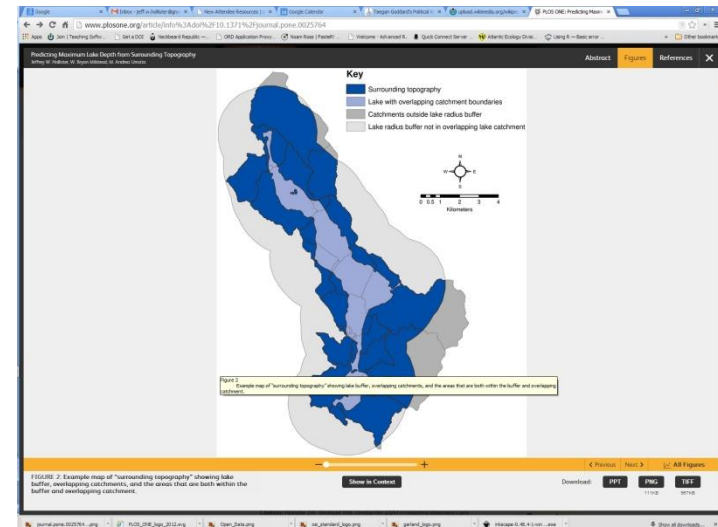
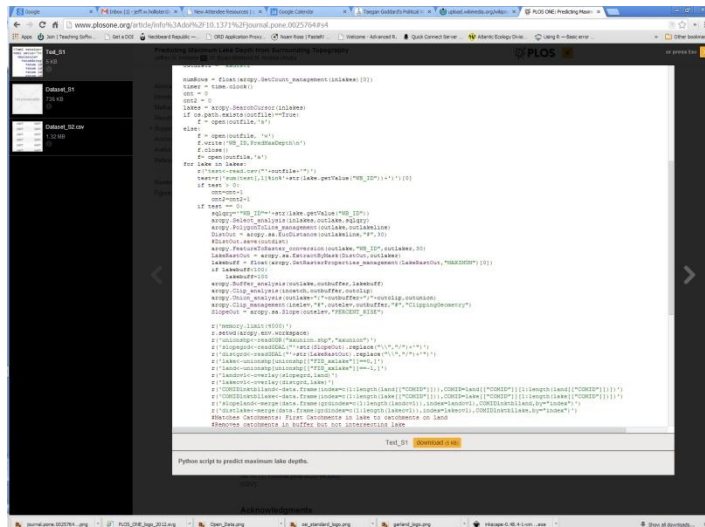
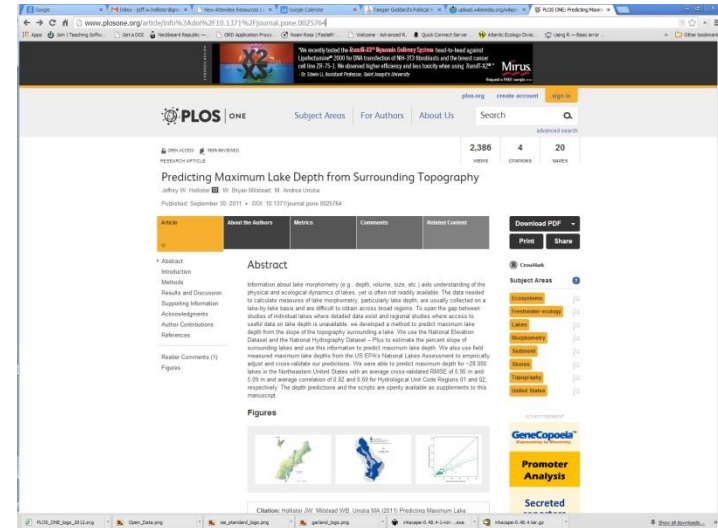
# Open Science and Our research

- Open Access
- Open Source
- Open Data



# Open Access: What we've done

- [Hollister et al, 2011](#)
- [Hilborn et al, 2013](#)
- [Milstead et al, 2013](#)



# Open Access: What's next?

- Goal: All publications open access
  - Journal choice (e.g. PeerJ, F1000Research, eLife, Frontiers In, etc.)
  - Funds to pay for OA charges in traditional journals

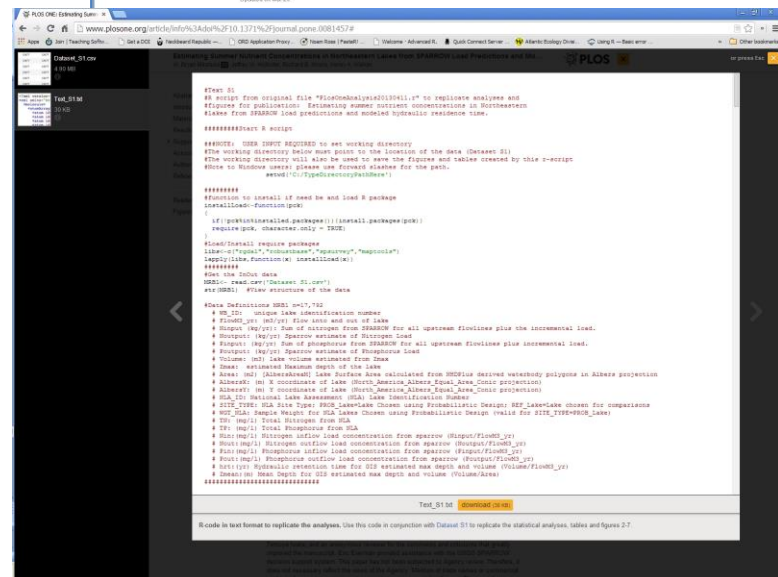
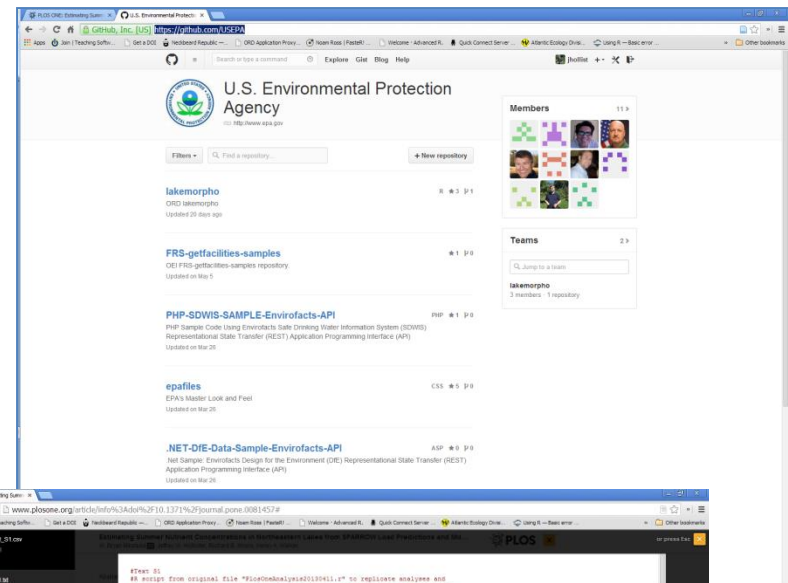


# Open Source: What we've done?

- Use Open Source
  - R, Python
- Supplemental Information
- Github



python



# Open Source: What Next

- Continued use of Github
  - R packages
  - manuscripts (e.g., [Ram, 2013](#))
  - posters/presentations (e.g., [@kbroman](#))
- Working with the community
  - Software Carpentry
  - Other groups



# Open Data: What we've done

- Supplemental Info
- Portals
  - EPA Environmental Dataset Gateway
  - APEX/Oracle

**EPA Environmental Dataset Gateway (EDG)**  
Connecting EPA's Environmental Resources

HOME ABOUT SEARCH BROWSE DATA REUSE RESOURCES

**Details Review Relationships**

**Lakes Ecosystem Services Download Package**

**Identification Information**

Title: Lakes Ecosystem Services Download Package  
Originator: US-EPA  
Publication: 20130515  
Date: 20130515

**Abstract:** This data download package contains Esri 10.0 MXDs, file geodatabases and copy of this FGDC metadata record. The data in this package are used in support of the Lake Ecosystem Services application available at the secondary linkage listed above. Layers contained in this data package are: polygons and centroids of lakes sampled as part of EPA's New England Lakes and Ponds project and the National Lakes Assessment project; CMAQ annual nitrogen deposition (2002) and nitrogen projections (2020); NASS Cropland Data Layer; USGS NHD; NLCD 2001; Omenik levels I, II and III ecoregions for the northeast region; 2010 census population for the northeast region in raster format; modeled nitrogen and phosphorus loads for NHD lakes in the USGS MRB1 region; and level 3 and level 9 Wadeable Streams Assessment ecoregions.

**Purpose:** The Lakes Ecosystem Services Online GIS provides geospatial visualization, query, and analysis tools. The Online GIS was built on the data collected as part of our research into ecosystem services in lakes. This includes information such as the National Lakes Assessment field data, USGS SPARROW results, National Land Cover Dataset, crop data, etc. With the various tools provided in the Online GIS, users can make and print maps from the datasets provided, query and display data with different cutpoints, conduct buffer analyses around lakes and summarize key datasets, and generate multi-variate radar graphs of water quality data.

Progress: Completed  
Frequency: None Planned

**Time Period of Content**

Single Date

**Lakes Ecosystem Services Database**

U.S. ENVIRONMENTAL PROTECTION AGENCY

Search Information Water Quality Science Links

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 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# Open Data: What's Next

- Linked Open Data
- Web APIs
  - Use HTTP
    - GET, POST, PUT, etc.
    - Access data
      - Programmatically
      - Machine-to-machine
  - rOpenSci: great example



An aerial photograph of a large body of water, likely a lake or a wide river, surrounded by dense green forest. Several small, forested islands and peninsulas are visible, creating a complex shoreline. The water is a deep blue color. The text "New England Monitoring" is overlaid in the center of the image.

# **New England Monitoring**



iOS Simulator – iPad / iOS 7.1 (11D167)

Carrier 11:05 AM 100%

<< State: Enter data Site ID: Enter data >>

NAME

SAMPLE LOCATION

PHYCO

METADATA

SUBMIT

iOS Simulator – iPad / iOS 7.1 (11D167)

Carrier 11:07 AM

>> State: Alaska Site ID: AK01 >>

### Type of sample and location

#### Within-lake:

Dist: 3 meters: ☒

Other (m): Enter data

Sample	Lat	Long	Time
WL-1:	123	234	Enter data
WL-2:	12	567	Enter data
WL-3:	12	Enter data	Enter data

#### Shore side:

Dist: 1 meter: ☒

Other (m): Enter data

Sample	Lat	Long	Time
SS-1:	Enter data	Enter data	Enter data
SS-2:	Enter data	Enter data	Enter data
SS-3:	Enter data	Enter data	Enter data

iOS Simulator – iPad / iOS 7.1 (11D167)

Carrier 11:06 AM 100%

>> State: Alaska Site ID: AK01 >>

Waterbody Name: Alaska test

Sampling Date: 07/08/2014

Name of samplers: Bill and ted

Weather conditions: Rainy and cloudy

Update DB

# Thank you!

# Questions?



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